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A SPECTROSCOPY OF HELIX MELTING(U) PURDUE UNIV
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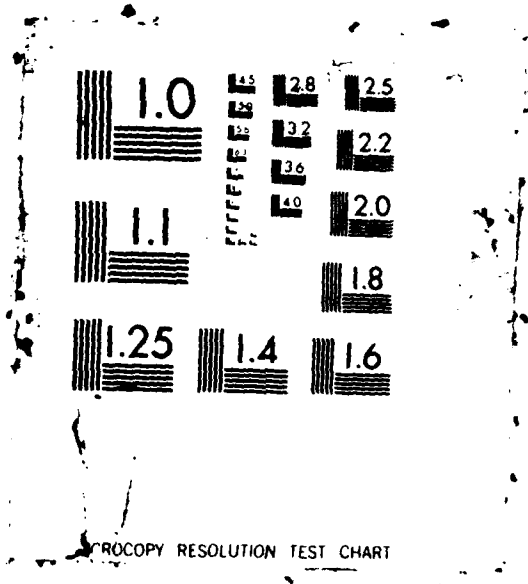
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PHOTOCOPY RESOLUTION TEST CHART

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19 ABSTRACT (Continue on reverse if necessary and identify by block number) We have calculated the dependences of the melting of poly(dG)-poly(dC) on vibrational mode excitation level. We find that bands of modes in the 10-100/ cm^{-1} range can alter details of helix melting. Melting is involved in important biological processes. The frequency range of this phenomenon is that of the Santa Barbara FEL. The SBFEL is an ideal device for exploration of this biological phenomenon. We are in collaboration with Prof. S. M. Lindsay's program which is an experimental exploration of the irradiation of DNA at SBFEL. (keyword)					
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Annual Report

A Spectroscopy of Helix Melting

N00014-86-K-0252

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Our effort is centered on calculations of DNA helix melting and the role of vibrational excitations in such melting. Our early results indicate that vibrational modes in the frequency range from $10 - 100 \text{ cm}^{-1}$ are the dominant element in bringing about helix melting. This frequency range is the same as that covered by the Santa Barbara Free Electron Laser Facility. It is the premier source of fine tuned radiant energy in this regime. We are calculating the expected helix behavior as these modes are excited presumably by FEL irradiation. The theoretical method we have developed indicated that several details of the helix melting were controlled by the excitation level of these vibrational modes.

By melting we mean the usual definition of DNA melting i.e., breaking up of the double helix into single strand DNA. The most fundamental processes such as RNA transcription and DNA replication require this form of melting, as it is essential to the reading of the base sequence message incorporated in the DNA. In these processes a small region of DNA is melted and this melt is propagated along the DNA so that whole genes can be read. The process must be carefully controlled and this control is a likely element of control of gene expression.

In our most sophisticated theoretical model we use a DNA homopolymer, poly(dG)·poly(dC), with a single base pair melted region. We monitor the elongation or propagation of such a melt by calculating the melting of adjacent base pairs. We find that the direction of propagation of the melt is controlled by the level of excitation of specific vibrational modes. Modes at $80 - 100 \text{ cm}^{-1}$ are particularly effective at advancing the melt along the $3' \rightarrow 5'$ direction in the G backbone. Modes below 20 cm^{-1} are particularly effective at advancing the melt in the opposite direction along the double helix. Not only is the direction of melt controlled by the level of vibrational excitation, but also the way in which the melting occurs is controlled by mode excitation. Those modes which cause melting to proceed $3' \rightarrow 5'$ along G also cause melting to originate at the major groove side of the DNA helix. Those modes that elongate the melt in the opposite direction induce melting to originate at the minor groove or opposite side of the helix. Our initial results therefore indicate that details of the melting process are a strong functions of details of the vibrational mode levels of excitation. These mode excitations may be influenced by FEL irradiation. The results quoted are published in J. Biomolec. Struct. and Dyn. 4, 437-442, (1986). A reprint is enclosed with this report.

A second effort during this year was the calculation of the behavior of these $10 - 100 \text{ cm}^{-1}$ modes with temperature down to very low temperature. Experimental data on the low temperature frequency shift became available from FTIR measurements made at the Max Planck Institute in Stuttgart. We have predicted frequency shifts in good agreement with those observed. This work has been

written up in preprint form and has been submitted for publication in Phys. Rev. B.

A preprint is enclosed with this report. The agreement is an indication that our calculations and parameters do correspond well to the DNA double helix.

More progress has been made during this first year but it has been along the line of formulating and coding further calculations for which results are not yet available. We are making progress on calculating the melting behavior of a greater range of DNA base compositions so as to better compare our theoretical results to the observations on FEL irradiation when such data becomes available. We are in close collaboration with Prof. S. M. Lindsay at Arizona State University who is involved in DNA irradiation experiments at the Santa Barbara FEL.

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